Macromolecular Crystallography

Summary of the July 18, 2007
Breakout Session

Beam line (s) - current resources

Most common beamline elements in use

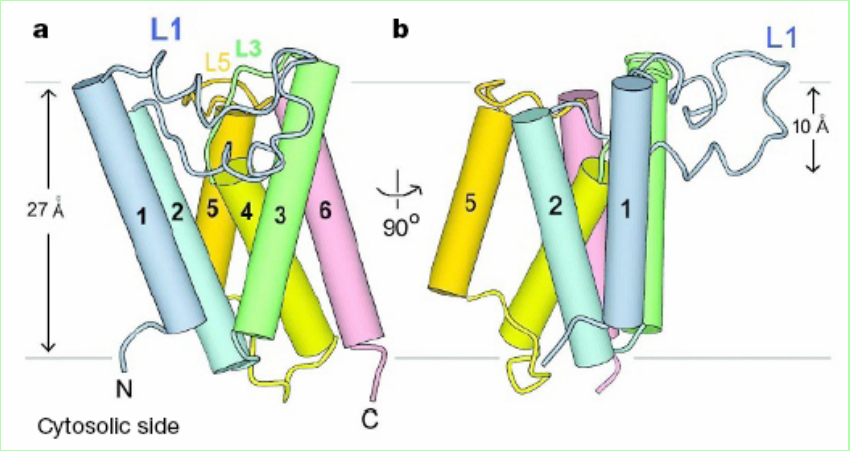
Optics

Source: Undulators; Wigglers
Monochromators: double crystal, sagital focusing, channel cut-Silicon
Mirrors: focusing, collimating; Kirk-Baez pairs
Energy range: 7 - 20 KeV

End-station

Diffractometers:Build In-house or Crystallogic (single axis, kappa); Hubbert; EMBL MicroDiffractometer*
Detectors: ADSC, MarCCD
Control: Blu(Web)ICE

Science Highlights



Beamlines: X6A, X29

Technique: Macromolecular Crystallography

Researchers:
Yongcheng Wang, Yingjiu Zhang and Ya Ha (Yale School of Medicine)

Publication:
"Crystal structure of a rhomboid family intramembrane protease" *Nature* (2006) 444, 179-180

What can be done with a new source such as NSLSII

Challenges

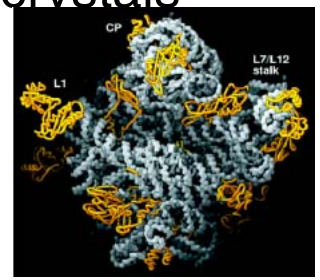
- Molecular Machines - multiple stage molecular machines
- Membrane Proteins
- Virus

- Structural "-omics"
- Drug development (vaccines, anesthetics…)

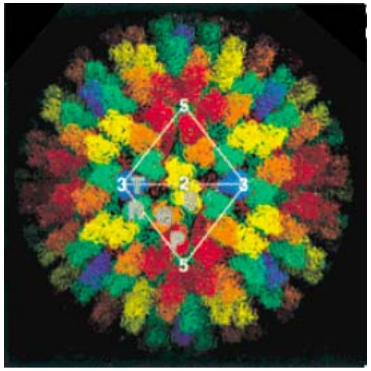
- Time resolved….kinetics….dynamics

- ✓Very small less then 10 micron or most probably smaller crystals
- ✓Weakly diffracting crystals

50 ang



250 ang



750 ang

My next Macromolecular Crystallography beam line(s)

Beam lines

Small beams, positional stability, small divergence, beam line automation.

Optics

Monochromator: Si 311
Mirror: KB mirrors (bimorph?)
Energy range: 3(2) to 60 keV

End-station

Large detectors, continuous read out preferred
Rotation axis with small sphere of confusion (< 1 micron)
Crystal visualization/centering tools (need research)
Ancillarydevices

My next Macromolecular Crystallography beam line(s)

Laboratories and ancillary facilities

Labs

- Wet labs,
  - cold rooms
  - microscopes
  - crystallization facilities (?)
  - Biohazard Level (?)
  - DI-water
- Mechanical, Electrical

IT

- remote user access
- security
  - e.g. through certificates
- large capacity data storage

Quality of Life

Facility

meeting rooms small and medium or convertible
offices for staff and visitors
lunch room for users and staff

Housing

short stay - hotel like
long stay - 1, 2, 3 Bedrooms with kitchen facilities

Food

vending automats - better setup then the vending machines
small convenience store (18/7)

Transportation

campus only
between BNL Stony Brook and Ronkonkoma train station (?)paid

IT

wireless network on campus